QCD simulations at small chemical potential*

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Within the reweighting approach, one has the freedom to choose the Monte Carlo action so that it provides a good overlap with the finite-μ measure but remains simple to simulate. We explore several choices of action in the regime of small μ. Simulating with a finite isospin chemical potential $\mu_I = \mu$ gives a better overlap than the standard choice $\mu = 0$, with no computational overhead.

1. INTRODUCTION

Because heavy ion collision experiments at RHIC correspond to a chemical potential μ as small as 10MeV, lattice QCD simulations at small μ have attracted renewed interest. To address the sign problem caused by the complex fermion determinant, three approaches have been proposed. (*i*) Analytically continuing results obtained at imaginary chemical potential [1]; (*ii*) Measuring the coefficients of the Taylor expansion of each observable about $\mu = 0$ [3,4]; (*iii*) Measuring the observables from a reweighted ensemble [5]. (*i*) trades the sign problem for that of the analytic continuation; the approach works well for smooth functions of μ [2]. We will not discuss it further here. (*ii*) has no sign problem, but rapidly becomes complicated as the Taylor order increases. (*iii*) is enjoying a successful revival in a two-parameter version, where results at (β, μ) are obtained by reweighting the $(\beta_0, \mu_0 = 0)$ simulation [6,7]. The accessible range of chemical potentials and volumes is still limited by the sign problem. But also, ensuring a sufficient overlap between the desired ensemble at (β, μ) and the Monte Carlo ensemble at $(\beta_0, \mu_0 = 0)$ is notoriously difficult. The acceptable shift of parameters normally decreases like 1/volume.

It seems useful then to consider the sampling of an approximate finite-μ action. Reweighting to the exact action will be mild and safe. The difficulty is to capture most of the exact measure, while avoiding the computation of the exact, complex determinant at each Monte Carlo step. We explore three variants of this strategy below.

2. SIMULATIONS AT SMALL μ

The QCD partition function with chemical potential, here for staggered quarks, is given by

$$Z(\mu) = \int dU \ \det M(\mu)^{\frac{n_f}{4}} \ \exp(-S_G) \qquad (1)$$

with S_G the gluon action and $M(\mu)$ the Dirac matrix. Writing $\det M(\mu) = |\det M(\mu)| \exp(i\hat{\theta})$ and defining $\theta \equiv \frac{n_f}{4}\hat{\theta}$, Eq.(1) becomes

$$Z(\mu) = \int dU \ |\det M(\mu)|^{\frac{n_f}{4}} e^{i\theta} \ \exp(-S_G). \qquad (2)$$

To allow Monte Carlo sampling over a positive measure, the expectation value of an observable $O(\mu)$ is recast into

$$\langle\ O(\mu)\ \rangle = \frac{\langle\ O(\mu)\ e^{i\theta}/f\ \rangle_{\tilde{Z}}}{\langle\ e^{i\theta}/f\ \rangle_{\tilde{Z}}} \qquad (3)$$

$\langle\ ..\ \rangle_{\tilde{Z}}$ means that the average is taken over configurations sampled from the partition function $\tilde{Z}$

$$\tilde{Z} = \int dU \ |\det M(\mu)|^{\frac{n_f}{4}} \ \exp(-S_G)\ f(U) \qquad (4)$$

where $f(U)$ is any positive functional of the gauge field. $e^{i\theta}/f$ is then the correction (reweighting)

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factor applied to each configuration. The standard strategy corresponds to $\tilde{Z} = Z(\mu = 0)$, i.e.

$$f \;=\; \left| \frac{\det M(\mu=0)}{\det M(\mu)} \right|^{\frac{n_f}{4}} \qquad (5)$$

One would like to find an optimal choice for $f(U)$. Setting aside the algorithmic issue of sampling a given $f(U)$, the optimal choice is that which maximizes the statistical accuracy on $\langle\, O(\mu)\,\rangle$ for an ensemble of N uncorrelated configurations. If $O(\mu)$ is not specified, it is reasonable to minimize the fluctuations in the reweighting factor, i.e. the relative error on the denominator of Eq.(3), since it propagates to all observables. From the central limit theorem, that error is, for N large

$$\frac{1}{\sqrt{N}} \sqrt{\langle\, (\frac{1}{f}\cos\theta)^2 \,\rangle / \langle\, \frac{1}{f}\cos\theta \,\rangle^2 - 1} \qquad (6)$$

This expression is minimized for

$$f \;=\; |\cos\theta| \qquad (7)$$

which reduces the denominator of Eq.(3) to the average sign $\langle\, \mathrm{sgn}\cos\theta \,\rangle_{\tilde{Z}}$. Therefore, it would be desirable to sample from

$$\tilde{Z}_{\rm opt} = \int dU \;|\det M(\mu)|^{\frac{n_f}{4}} \;|\cos\theta| \;\exp(-S_G) \qquad (8)$$

The drawback of this sampling choice is that the phase θ of $\det M(\mu)$ must be evaluated at each Monte Carlo step, at a computational cost $\propto L^9$ for a lattice of size $L^3 \times N_t$. Thus, this strategy seems prohibitively inefficient. We consider three alternatives, which can be implemented at reduced computing cost and are closer to the optimal choice Eq.(7) than the standard Eq.(5).

• **Method A:** $f = 1$

The sampling measure is $\propto \det{}^{\frac{n_f}{8}}[M^\dagger(\mu)M(\mu)]$. Since $\det M^\dagger(\mu) = \det M(-\mu)$, this amounts to simulating a finite *isospin* chemical potential [8] $\mu_I = \mu$. Compared with the standard sampling measure $\propto \det{}^{\frac{n_f}{4}} M(\mu = 0)$, this method captures, with no computational overhead, the fluctuations of the magnitude of the determinant which may account for a good part of the relevant physics at small μ. Indeed, the critical line $T_c(\mu)$ in the isospin-μ case seems to have a similar curvature as in the usual isoscalar-μ case [9].

$f(U)$	$\mu = 0.1$	0.15	0.20	0.25	0.30
Eq.(5)	0.089	0.22	0.45	0.97	2.67
1	0.085	0.17	0.33	1.08	3.83
$e^{-\bar{\theta}^2/2}$	0.017	0.09	0.46	2.21	15.8
$\lvert\cos\bar{\theta}\rvert$	0.008	0.05	0.46	14.4	14.2

Table 1
Standard deviation (numerator Eq.(6)) of the reweighting factor $\cos\theta/f$ as a function of μ, for various sampling choices $f(U)$. This number is proportional to the relative error on a smoothly varying observable, for a given statistics. The top line is the standard choice.

To verify the improvement of the overlap with the desired measure, we generated ensembles of 200 configurations ($\beta = 4.8, n_f = 2, ma = 0.025, 4^4$ lattice), using the standard method ($\mu = 0$) and using method A, i.e. at isospin $\mu_I \neq 0$. Reweighting was then performed on each ensemble to obtain results at isoscalar chemical potential $\mu = \mu_I$. Fluctuations of the reweighting factor were measured by the numerator of Eq.(6). Table 1 shows that, for small μ, the standard method (1rst line) gives larger fluctuations, i.e. a poorer sampling, than method A (2nd line).

Still, in either method the factor $\cos\theta$ must be computed for each configuration in the ensemble. For small μ, it is possible to approximate θ by its truncated Taylor expansion:

$$\begin{aligned} \theta \;&=\; \frac{n_f}{4}\mathrm{Im\ Tr\ log}\, M(\mu) = \bar{\theta} + \mathcal{O}(\mu^3), \\ \bar{\theta} \;&\equiv\; \frac{n_f}{4}\;\mu\;\mathrm{Im\ Tr}\; M^{-1}\dot{M}\Big|_{\mu=0} \end{aligned} \qquad (9)$$

where $\dot{M} \equiv \dfrac{\partial M}{\partial \mu}$. The advantage is that the trace can then be estimated using n noise vectors η_i as

$$\mathrm{Tr}\; M^{-1}\dot{M} \approx \frac{1}{n}\sum_i^n \eta_i^\dagger\; M^{-1}\dot{M}\;\eta_i. \qquad (10)$$

This approach has been used in [7], with $n = 10$, on a $16^3 \times 4$ lattice. To test the quality of this approximation, we measured the exact phase θ and its linearized approximation $\bar{\theta}$ on each configuration of our isospin-μ gauge ensembles. The scatter plot Fig. 1 shows that the correlation between θ and $\bar{\theta}$ is excellent at $\mu = 0.1$ (i.e. $\mu/T = 0.4$),

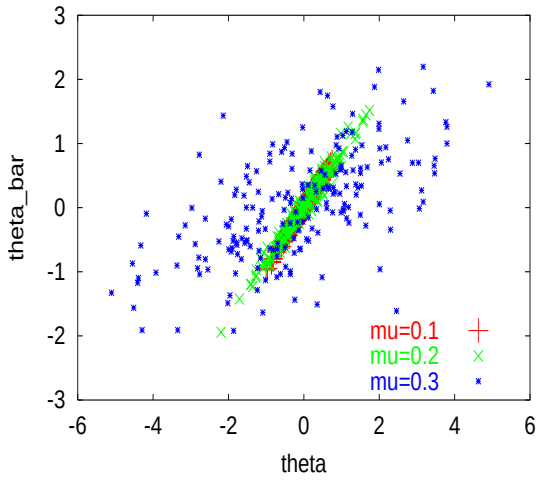

Figure 1. The linearized phase $\bar{\theta}$ of the determinant vs the exact phase θ, for 3 values of μ.

and very poor at $\mu = 0.3$. One may expect this correlation to persist for larger volumes. Therefore, using the linearized approximation $\bar{\theta}$ up to $\mu/T \sim 0.4$, as advocated in [7], appears justified. On the other hand, the stochastic estimator of $\bar{\theta}$ Eq.(10) was extremely noisy and required several thousand noise vectors.

• **Method B:** $f = e^{-\frac{1}{2}\bar{\theta}^2}$

To approach the optimal $f = |\cos\theta|$ at small μ without computing higher derivatives in the Taylor expansion Eq.(9), one can use $\cos\theta \approx 1 - \frac{1}{2}\bar{\theta}^2 \approx \exp(-\frac{1}{2}\bar{\theta}^2)$. The additional term $S_{\bar{\theta}} = \frac{1}{2}\bar{\theta}^2$ in the action can be included in an R-type algorithm [10], where the Tr log is estimated at each step using noise vectors. Here, two uncorrelated noise vectors are necessary to estimate $\bar{\theta}^2$. Maintaining the $\delta\tau^2$ accuracy of the R-algorithm in the stepsize seems less obvious, but may be feasible.

To assess the advantages of method B over method A, we compare in Table 1 the standard deviation of the reweighting factor $\cos\theta/f$. A large reduction is seen at small μ.

• **Method C:** $f = |\cos\bar{\theta}|$

To approach $|\cos\theta|$ even better at small μ, one may consider the choice $f = |\cos\bar{\theta}|$. As above, $\bar{\theta}$ can be estimated via Eq.(10). Then, an unbiased estimator of $\cos\bar{\theta}$ can be formed by a stochastic Taylor expansion as in [11], which can be used in the Monte Carlo update. As long as $\cos\bar{\theta}$ remains positive, i.e. for small μ, an important gain is possible as seen in Table 1.

3. CONCLUSIONS

We have considered three choices of Monte Carlo actions which can be used to obtain finite-μ results after reweighting. Compared to the standard choice of simulating at $\mu = 0$, they provide better statistical accuracy at small μ ($\mu/T \lesssim 0.5$), because the reweighting factor fluctuates less. In the case of Method A (isospin chemical potential $\mu_I = \mu$), this improvement is achieved with no computational overhead. Moreover, results at finite μ_I come for free.

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